APPENDIX B

MATHEMATICAL MODELING

B-1. Introduction.

a. Models. Three types of models are pertinent in the investigation of the environmental impact of deepening navigation channels:

(1) Hydrodynamic models which describe the velocity and salinity distributions within the study area.

(2) Water quality models which predict physical characteristics and chemical constituent concentrations of the water at various locations within the study area.

(3) Ecological models which predict the interactions between water quality and the aquatic community.

b. Database. The information derived from hydrodynamic models forms part of the database for water quality and ecological models, and the data from water quality models form part of the database for ecological models. Hence, it is essential that these foundation modeling activities be accomplished with adequate accuracy. The various models described require input data which may be classified as:

(1) Data that describe the initial state of the system.

(2) Data that describe the "boundary conditions" of the system. These data include system geometry and the quantity and constituent concentrations of freshwater inflows.

(3) Other data necessary for the calibration of the models, including a description of the hydrography of the study area. Because no model study can be more accurate than the information on which it is based, the importance of adequate field data cannot be overemphasized.

B-2. Field Data. The first steps in any model study must be the specification of objectives; an assessment of the geophysical, chemical, and biological factors involved; and collection of data essential to describe these factors. Assessment and data collection should include:

a. Identification of freshwater inflow sources, including their average, range, and time distribution of flow.

b. Assessment of the tides and currents that are anticipated within the region.

c. Assessment of wind effects and other geophysical phenomena that may be peculiar to the specific study.

d. Identification of the sources of sedimentation and of sediment types.

e. Identification of sources and the expected quantities and composition of industrial and municipal effluents, nonpoint contaminants, and tributary constituent concentrations.

f. Identification of the aquatic community of the region and the chemical, physical, and biological factors which influence its behavior.

g. Identification of the available hydrographic and other geometric data pertinent to preparation of the model.

The purpose of the preliminary assessment of pertinent and available data is to provide a basis for the selection of the models needed and to provide a basis for planning field data acquisition programs. The most satisfactory procedure is to plan the numerical modeling and field data acquisition program together. If possible, the basic hydrodynamic model should be operational during the period in which field data are being obtained. One major reason for concurrent model simulation and data acquisition is that anomalies in field data frequently occur, and the numerical model may be used to identify and resolve them.

B-3. Data Requirements. Data that are typically needed for hydrodynamic models include time history measurements of water surface elevations, velocities, and salinities. In conjunction with the field data acquisition program and the projected numerical modeling activity, a program of data analysis must be undertaken. For the data analysis program to be as efficient as possible, the field data should be recorded on media that can be automatically read by the computer equipment used in processing.

B-4. Data Analysis.

a. Elements. Data analysis includes isolation of the astronomical tide from the tidal record and an identification of the constituents of the astronomical tide. The purpose of separating the astronomical tide from the observed tide is twofold:

(1) This separation allows one to examine the residual and, by using statistical methods, to investigate the extent to which other geophysical phenomena, such as wind, influence the observed flow.

(2) The astronomical tide is deterministic and may be used in synthesizing tidal records for extreme and unusual events or during periods for which tidal records are not available.

b. Observations. Two observations need to be considered:

(1) The astronomical tide is somewhat dependent on freshwater inflows into the study region, and the amplitude of the tidal constituents therefore tends to vary seasonally in many coastal areas.

(2) Past experience in the analysis of tidal data in conjunction with model studies has shown that a minimum of about 30 days of record for tidal elevation, velocity, and salinity data is essential for satisfactory analysis.

B-5. Hydrodynamical Models.

a. General. Numerical models of hydrodynamic and water quality processes are said to be coupled if they are run simultaneously and interactively on a digital computer. If, conversely, the hydrodynamic model was run and the output from it used as input to the water quality model, the two models would be said to be uncoupled. In many instances it is more economical to run uncoupled models. Uncoupled models are unacceptable where thermal gradients or the concentration of dissolved or suspended material causes a large enough variation in the fluid density to substantially affect the flow. The various numerical models may be classified as one-, two-, or three-dimensional. The one-dimensional models treat the system by averaging over a succession of cross sections. One-dimensional models are well suited to geometric situations such as channels with relatively uniform cross-sectional shapes and center lines whose radius of curvature is relatively large compared with the width, provided the water density is uniform over the cross section. Two-dimensional models may be either depth or breadth averaged. Two-dimensional depth-averaged models are the type most commonly employed and are well suited to studies in areas such as shallow estuaries, where the water column is relatively well mixed. Breadth-averaged models are used in studies of relatively deep and narrow bodies of water with significant variation of density vertically through the water column. Three-dimensional models are relatively new and have been used in only a very limited number of practical studies. In general, two-dimensional models are substantially more expensive to run than one-dimensional models, and three-dimensional models are much more expensive than two-dimensional models. Hence, in situations where it is known that one of the simpler models will produce satisfactory results, the simpler model should be employed for economy.

b. Two-Dimensional Depth-Averaged Models. Two-dimensional depth-averaged models are most commonly employed in the investigation of tidal flows in inlets, bays, and estuaries. Two distinctly different formulations have been employed: finite difference and finite element. Models currently used at WES are mentioned briefly below. The finite difference model, WIFM (WES Implicit Flooding Model) evolved from early work by Leendertse (1967). The model and its application have been described at different stages of development by Butler (1979). The finite element flow model of Research Management Associates (RMA-2) (King and Norton 1978) evolved from work by Norton et al. (1973) sponsored by Walla Walla District. The WES version of this model and a companion sediment transport model, STUDH, and their application to project studies have been described by McAnally et al. (1984). A user's manual (US Army Engineer Waterways Experiment Station 1984) for these finite element models and support programs (system called TABS-2) is nearing completion. Most existing finite difference models employ Cartesian coordinates which, even with variable grid spacing capabilities, may lead to undesirable approximations in schematization of complex study areas. Recent work by Johnson (1980) has resulted in a finite difference model (VAHM) for flow and transport which employs a generalized coordinate transformation technique called boundary-fitted coordinates to overcome this limitation. Development of this approach is continuing.

c. Two-Dimensional Breadth-Averaged Models. Breadth-averaged models are applicable in studies of relatively deep, narrow channels with small radii of curvature in which lateral secondary currents of appreciable magnitude do not develop. Since fewer systems meet this criterion, work on models of this type has been more limited than on the depth-averaged models. However, work over the last few years has produced a useful model, LAEM (Laterally Averaged Estuarine Model) (Edinger and Buchak 1981). This model has been used to investigate the effect of navigation channel deepening on salinity intrusion in the Lower Mississippi River.

d. Three-Dimensional Models. Breadth- and depth-averaged two-dimensional models obviously lack the ability to predict secondary flows involving the plan that has been averaged. In some instances, these secondary currents may be appreciable and affect such things as salinity intrusion, sediment transport, thermal distribution, and water quality. Leendertse et al. (1973) pioneered the development of one of the early three-dimensional models of an estuary. Leendertse's model employed Cartesian coordinates. A three-dimensional model that uses "stretched coordinates" in both the horizontal and vertical dimensions has been developed and was applied in preliminary studies of the Mississippi Sound (Sheng and Butler 1983). Research level three-dimensional versions of the finite element flow and sediment models have also been developed and are being evaluated (Ariathurai 1982 and King 1982). Improvements in the efficiency of computational equipment and modeling technology are increasing the feasibility of applying three-dimensional models. Such models are, however, on the experimental frontier of what may reasonably be done with numerical models.

B-6. Water Quality Models.

a. General. Historically, the analysis of water quality has concentrated on the dissolved oxygen (DO) and biochemical oxygen demand (BOD). The balance between DO and BOD concentrations was the result of two processes: the reaeration of the water column, and the consumption of DO in oxidation of BOD. Later emphasis has been on extending and refining the Streeter-Phelps formulation by using a more generalized mass balance approach and by the inclusion of additional processes such as benthic oxygen demand, benthic scour and deposition, photosynthesis and respiration of aquatic plants, and nitrification. The more comprehensive water quality models have been developed to include the nitrogen and phosphorus cycle and the lower trophic levels of phytoplankton and zooplankton. A number of investigations have modeled the algal nutrient silica. Selected chemical constituents have been modeled by assuming thermodynamic equilibrium. The fate of toxicants such as pesticides, metals, and PCBs is very complicated involving adsorption-desorption reactions, flocculation, precipitation, sedimentation, and biological uptake. Examination of toxicants and their impact on biological populations requires ecological models. Selection of a water quality methodology requires consideration of the following:

(1) Water quality constituents.

(2) Dimensional and temporal resolution.

(3) Data requirements.

b. Water Quality Constituents. The water quality constituents most frequently simulated include salinity, light, temperature, DO, BOD, coliform bacteria, algae, nitrogen, and phosphorus. Each of these constituents interacts with the others, but the significance of their dependencies varies among constituents, and their inclusion in a numerical water quality model depends upon the study objectives and the water body under consideration. The environmental impact analysis of most deep-draft navigation projects can use salinity and DO as indices of environmental change.

(1) Salinity plays a dominant role in physicochemical phenomena such as focculation of suspended particulates, is used as a variable to define the habitat suitability for aquatic organisms, and is frequently employed as a conservative tracer to calibrate mixing parameters.

(2) Dissolved oxygen is a respiratory requirement for most organisms and is used as a measure of the "health" of aquatic systems. Dissolved oxygen can be used to evaluate the environmental significance of stratification resulting from channel deepening and realignment.

c. Dimensional and Temporal Resolution. In a numerical water quality model the choice is between a one-dimensional model and one that incorporates two or three spatial dimensions. A long, narrow, and vertically well-mixed water body may be represented by a one-dimensional model consisting of a series of segments averaged over the cross section. Where there is pronounced vertical stratification, it is likely that a laterally averaged two-dimensional model will be needed. In other situations where there are marked lateral heterogeneities in water quality but the water body is well mixed, a vertically averaged two-dimensional model is indicated. If significant lateral heterogeneities are accompanied by pronounced stratification, a three-dimensional model may be required. Most existing water quality models are one-dimensional. Practical applications of two-dimensional depth- and breadth-integrated models have been made and are feasible. Three-dimensional water quality models are presently research tools; data requirements for calibration and verification make them prohibitively expensive at present for practical application. The basis of all water quality models is a velocity field either specified by empirical measurements or computed by numerical hydrodynamic models. The current trend in hydrodynamic modeling is toward development of three-dimensional models with increased spatial and temporal resolution in order to resolve important scales and to minimize the need for parameterization. As a result, modern time-dependent hydrodynamic models normally have time steps on the order of minutes to one hour. The chemical and biological equations of water quality models have characteristic time scales determined by the kinetic rate coefficients. These time scales are usually on the order of one to ten days. The phenomena of interest, such as depletion of DO and excessive plant growth, occur on time scales of days to several months. Direct coupling of hydrodynamic and water quality models provides potential spatial and temporal resolution that cannot be effectively interpreted. The reasons are that present field sampling programs resolve constituent concentrations on the order of a kilometer to tens of kilometers in the horizontal, meters in the vertical, and days to weeks in time. In addition, the kinetic rate coefficients presently used in water quality models resolve dynamics on the order of days to weeks. Direct coupling substantially increases the cost of computation. Direct coupling is necessary only for those constituents such as temperature, salinity, and suspended particulates, whose contribution to density gradients may substantially affect the flow. Uncoupling permits averaging of the hydrodynamic model output, which results in less costly water quality computations.

B-7. Ecological Models. Ecological models include numerous biological species and emphasize food chain and species interactions. Ecological models are appropriate for addressing toxicants such as pesticides, metals, and PCBs and evaluating small incremental changes in nutrients, suspended particulates, and temperature. No general ecological model exists. Existing ecological models are site specific, dependent upon the local aquatic community, and specific to the toxicant of concern. The Environmental Laboratory at WES serves as a clearinghouse for Corps inquiries, and plans to become an active participant in ecological model application.

B-8. Modeling Systems. In this appendix, consideration has been given to some of the more important aspects of numerical model selection and application. Hydrodynamic, water quality, and ecological models may not be considered as individual entities. As explained, the various models must be coupled, or the output of one model must be used as input to a subsequent model. If the applicable models are to be used efficiently and economically, the data transfer between the models must be considered and steps must be taken to ensure output-to-input compatibility. In modeling there are, in addition to the modeling itself, data to be collected, analyzed, and put into appropriate databases. Each of these activities requires substantial data processing, and the aggregate cost of these activities may far exceed the cost of the actual modeling exercise. Also associated with most studies are other requirements, such as reports, which lead to additional data processing for such activities as computer graphics. The development of the models and other programs requires a broad spectrum of technical talents, and the execution of a comprehensive study may require the interaction of several individuals. What is essential to an effective study is a comprehensive, integrated system of modeling and utility programs, which is documented to the extent that the system may be understood and used by the various individuals participating in the study. Such systems are beginning to emerge. The WES Hydraulics Laboratory has developed a system for Open Channel Flow and Sedimentation (TABS-2) which uses depth-averaged finite element models to predict hydrodynamics, salinity, and sediment transport. The WES Environmental Laboratory is incorporating mass transport equations which include the chemical reaction terms in the two-dimensional, depth-averaged model WIFM (paragraph C-5), the transport portion of the boundary-fitted coordinate model VAHM (paragraph C-5), and the two-dimensional, breadth-averaged model LAEM (paragraph C-5). The emergence of such systems is a significant aspect of the advancement of numerical modeling.